Clustering in Fisher discriminative subspaces

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Abstract. Clustering in high-dimensional spaces is nowadays a recurrent problem in many scientific domains but remains a difficult problem. This is mainly due to the fact that high-dimensional data usually live in low-dimensional subspaces hidden in the original space. This paper presents a model-based clustering approach which models the data in a discriminative subspace with an intrinsic dimension lower than the dimension of the original space. An estimation algorithm, called Fisher-EM algorithm, is proposed for estimating both the mixture parameters and the discriminative subspace. Experiments show that the proposed approach outperforms existing clustering methods and provides a useful representation of the high-dimensional data.

Keywords: Model-based clustering, dimension reduction, discriminative subspaces, latent mixture model.

1 Introduction

In many scientific domains, the measured observations are nowadays high-dimensional and clustering such data is a challenging problem. Indeed, the most popular clustering methods are based on the Gaussian mixture model and show a disappointing behavior in high-dimensional spaces. They suffer from the well-known *curse of dimensionality* [1] which is mainly due in clustering to the specificities of high-dimensional data. On the one hand, high-dimensional data have intrinsic dimension lower than the dimension of the original space and, on the other hand, they can be noisy.

Since the dimension of observed data is usually higher than its intrinsic dimension, it is theoretical possible to reduce the dimension of the original space without loosing any information. Therefore, dimension reduction methods are traditionally used before the clustering step. Feature extraction methods such as Principal Component Analysis (PCA) [2] or feature selection methods (see [3] for a review) are very popular. However, these methods of dimension reduction do not consider the classification task and provide a sub-optimal data representation for the clustering step. Only few approaches combine dimension reduction and classification. Fisher Discriminant Analysis (FDA) (see Chap. 4 of [4]) is one of them in the supervised classification framework. FDA is a powerful tool for finding the subspace which best discriminates the groups and reveals the structure of the data. This subspace is

spanned by the discriminative axes which maximize the ratio of the between class variance and the within class variance.

This work proposes a method which adapts traditional procedures of clustering based on the Gaussian Mixture Model (GMM) for modeling and classifying data in discriminative subspaces. The approach proposed in this paper has three main objectives: firstly, it aims to improve clustering performances with the use of discriminative subspaces, secondly, it avoids estimation problems linked to high dimensions and, finally, it provides a low-dimensional discriminative representation of the data.

2 Model-based clustering in discriminative subspaces

The main idea of our approach is that real data live in a latent subspace with an intrinsic dimension lower than the dimension of the observed data and that a subspace of $K-1$ dimensions is theoretically sufficient to discriminate K groups. We therefore propose to model and classify the data in a discriminative subspace with $K-1$ dimensions. The proposed approach will thus provide an optimal partition of the data as well as a discriminative representation of the partition.

2.1 The latent mixture model

Clustering aims to divide a given dataset of n observations $\{y_1, \ldots, y_n\}$ into K homogeneous groups (see [5] for a review). In this work, the observed data $\{y_1, \ldots, y_n\} \in \mathbb{R}^p$ are assumed to be a linear transformation of latent (non observed) data $\{x_1, \ldots, x_n\} \in \mathbb{R}^d$:

$$y = x\ V + \epsilon,$$

where $x \in \mathbb{R}^d$, $y \in \mathbb{R}^p$, $d < p$, V is the $d \times p$ transformation matrix and $\epsilon \in \mathbb{R}^p$ is a noise term. Popular clustering techniques use Gaussian Mixture Models (GMM), which assume that each class is represented by a Gaussian probability density. Let us therefore assume that the data $\{x_1, \ldots, x_n\}$ are independent realizations of a random vector $X \in \mathbb{R}^d$ with density function f:

$$f(x) = \sum_{k=1}^{K} \pi_k \phi(x, \theta_k),$$

where K is the number of clusters, ϕ is the Gaussian density function parameterized by $\theta_k = (\mu_k, \Sigma_k)$, and π_k, μ_k and Σ_k are respectively the proportion, the mean and the covariance matrix of the kth component of the mixture.

2.2 Estimation procedure: the Fisher-EM algorithm

The parameters of a mixture model are usually estimated by the maximum likelihood method through the iterative Expectation-Maximization (EM) algorithm [6]. Since, in this work, the data are not modelled in the space of observed data but in a latent subspace of dimension $d < p$, the estimation procedure has to be modified to take into account these specificities. Due to the nature of the model described above, the estimate procedure alternates between three steps: an E-step in which posterior probabilities of each observation are computed, a F-step which estimates the inverse transformation conditionally to the posterior probabilities and a M-step in which parameters of the mixture model described in the latent subspace of dimension d are determined by maximizing the conditional likelihood. This estimation procedure, called hereafter Fisher-EM algorithm, has the following form:

E-step: This step computes, at each iteration (q), the posterior probabilities t_{ik} that an observation belongs to the kth component of the mixture (in the subspace of dimension d):

$$t_{ik}^{(q)} = \frac{\pi_k^{(q-1)}\phi(x_i, \theta_k^{(q-1)})}{\sum_{k=1}^{K} \pi_k^{(q-1)}\phi(x_i, \theta_k^{(q-1)})},$$

where ϕ is the Gaussian density, and $\pi_k^{(q-1)}$ and $\theta_k^{(q-1)}$ are the parameters of the kth mixture component estimated in the latent subspace at the previous iteration.

F-step: At the iteration (q), this step computes the discriminative axes, so-called Fisher axes, by estimating the inverse transformation conditionally to the posterior probabilities t_{ik}. These axes are determined by maximizing the ratio of the between-class variance and the within-class variance. According to the Huygens' theorem, this optimization problem resumes to:

$$max_u \frac{u^t B^{(q)} u}{u^t S u},$$

where $S = \frac{1}{n}\sum_{i=1}^{n}(y_i - m)^t(y_i - m)$ and $m = \frac{1}{n}\sum_{i=1}^{n} y_i$ are respectively the covariance matrix and the mean of the observed data, and:

$$B^{(q)}(t_{ik}) = \frac{1}{n}\sum_{k=1}^{K} n_k^{(q)}(m_k^{(q)} - m)^t(m_k^{(q)} - m),$$

$$n_k^{(q)} = \sum_{i=1}^{N} t_{ik}^{(q)},\ m_k^{(q)} = \frac{1}{N}\sum_{i=1}^{N} t_{ik}^{(q)} y_i\ .$$

The solutions of this optimization problem are the eigenvectors associated to the $K-1$ largest eigenvalues of the matrix $S^{-1}B^{(q)}$.

M-step: This step estimates the parameters of the mixture model by maximizing the conditional likelihood: the prior probabilities π_k, the means μ_k and the covariance matrix Σ_k of the K components in the space of the Fisher discriminative axes:

$$\mu_k^{(q+1)} = \frac{\sum_{i=1}^N t_{ik}^{(q)} x_i^{(q)}}{\sum_{i=1}^N t_{ik}^{(q)}},\ \pi_k^{(q+1)} = \frac{\sum_{i=1}^N t_{ik}^{(q)}}{N}$$
$$\Sigma_k^{(q+1)} = \frac{\sum_{i=1}^N t_{ik}^{(q)} (x_i^{(q)} - \mu_k)^t (x_i^{(q)} - \mu_k)}{\sum_{i=1}^N t_{ik}^{(q)}},$$

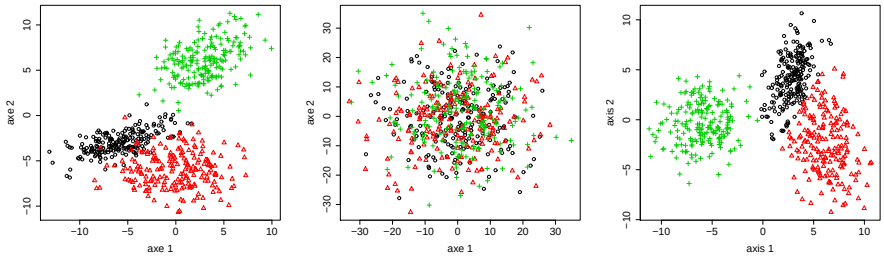
with $x_i^{(q)} = y\, U^{(q)}$ where $U^{(q)}$ is the $p \times d$ inverse transformation matrix which contains the eigenvectors associated with the d largest eigenvalues of $S^{-1}B^{(q)}$. Traditionally, such an estimation approach on high-dimensional data yields to problems for estimating the mixture model parameters. Conversely, the current approach computes very few parameters since their estimates are determined in a subspace of dimension $d = K - 1$ smaller than the dimension of the original space, and independent from the dimension of the original space.

3 Experimental results

In this section, the Fisher EM algorithm is applied on simulated data. The following experiments aim to highlight the main features of the proposed clustering method: visual representation and clustering performance in high-dimensions.

3.1 Visual representation of the partition

For this first experiment, 600 observations have been simulated following the mixture model considered in the previous section. The simulated dataset is made of 3 groups and each group is modeled by a Gaussian density in a 2-dimensional space completed by 23 dimensions of Gaussian noise. Figure 1(a) shows the simulated data in their 2-dimensional latent space whereas Figure 1(b) presents the projection of the 25-dimensional observed data on the two first principal components of PCA. As we can observe, the PCA representation of the data is actually not well suited for clustering these data even so it exists a representation which discriminates perfectly the three groups. Figure 1(c) shows the partition provided by the Fisher-EM algorithm on the estimated discriminative subspace. On the one hand, the result of the Fisher-EM algorithm appears to be a very informative representation. On the other hand, the partition provided by the Fisher-EM algorithm is an optimal partition (96% correct) since it equals the Bayes' classifier (computed with the true densities).



(a) Data in the latent space. (b) Projection on 2 axis of PCA. (c) Estimated Fisher axis.

Fig. 1. Clustering of simulated data $\in \mathbb{R}^{25}$ with an intrinsic dimension equals to 2.

3.2 Effect of the dimension

This second experiment aims to compare on a simulated dataset the performances of the Fisher-EM algorithm with traditional clustering methods such as the classical EM algorithm, the EM algorithm calculated on the principal components of PCA (hereafter PCA+EM) and the k-means algorithm. As before, the simulated dataset is made of 3 groups where each group is modeled by a Gaussian density in a 2-dimensional space completed by 1 to 15 dimensions of Gaussian noise. The same initial conditions have been used for each method and we have chosen, for this study, an initialization on parameters proposed by McLachlan and Peel [7]. Finally, the experiment has been repeated 20 times in order to average the classification results. Figure 2 presents the effect of the dimension on the classification performances obtained with Fisher-EM, EM, PCA+EM and k-means. Firstly, the performances of EM and PCA+EM algorithms decrease proportionally when the dimension increases. Secondly, k-means algorithm has a lower performance than other methods in the initial space and becomes worse when the dimension increases. Finally, the dimension appears to have no significant influence on the Fisher-EM performances. The correct classification rate is 0.90 on average whatever the dimension is. However, Fisher-EM turns out to have the same weakness as the EM algorithm: it has a slight instability due to the initial conditions. Nevertheless, the correct classification rate of the Fisher-EM algorithm remains very satisfying for the whole range of dimensions.

4 Conclusion

In this work, a model-based clustering method in Fisher discriminative subspaces has been proposed. This approach is based on a latent mixture model in a discriminative subspace. An EM-like estimation procedure, called Fisher-EM algorithm, is proposed to estimate both the discriminative subspace and

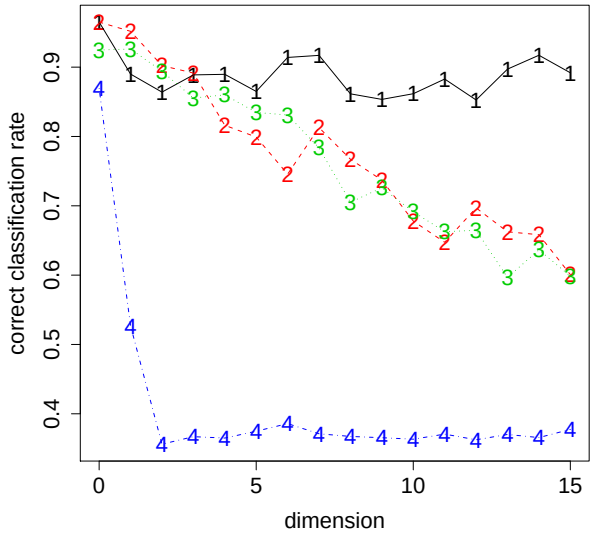


Fig. 2. Influence of the dimension on the correct classification rate for Fisher-EM (1-black), EM (2-red), PCA+EM (3-green) and k-means (4-blue).

the mixture model parameters. Experiments on simulated data have shown that the proposed approach outperforms traditional clustering methods and that the Fisher-EM algorithm seems not sensitive to high dimensions. Moreover, the proposed latent mixture model is parsimonious since the number of estimated parameters is independent of the initial dimension of the data. Finally, this approach provides as well a comprehensive representation of the structure of high-dimensional data.

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